

Two-dimensional negative donors in magnetic fields

Mikhail V. Ivanov* and Peter Schmelcher†

*Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg,
INF 229, D-69120 Heidelberg, Federal Republic of Germany*

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A finite-difference solution of the Schrödinger equation for negative donor centers D^- in two dimensions is presented. Our approach is of exact nature and allows us to resolve a discrepancy in the literature on the ground state of a negative donor. Detailed calculations of the energies for a number of states show that for field strengths less than $\gamma = 0.117a.u.$ the donor possesses one bound state, for $0.117 < \gamma < 1.68a.u.$ there exist two bound states and for field strengths $\gamma \geq 1.68a.u.$ the system possesses three bound states. Further relevant characteristics of negative donors in magnetic fields are provided.

I. INTRODUCTION

The properties of D^- centers in narrow quantum wells have become a subject of considerable interest during the past years^{1,2,3,4,5,6,7,8,9}. In very narrow wells this system can be considered as a two-dimensional counterpart of the atomic H^- ion. A frequently used compound for current experimental investigations (see for example ref.¹⁰) of such systems are layers of GaAs/AlGaAs. The high mobility i.e. small effective mass of the electrons and the comparatively large dielectricity constant of this semiconductor material allow us to study strong magnetic field effects in the laboratory. Both the two-dimensional character of the motion of the electrons and the external magnetic field makes the ground state of the system more tightly bound than that of the field-free three-dimensional H^- ion. Considering neutral donors D^0 the planar electron density of the 2d donor is enhanced significantly compared to that of the 3d donor. The form of the corresponding charge distribution makes the interaction of an additional distant charge with the neutral donor very different for the three-dimensional compared to the two-dimensional situation. In three dimensions it is well-known that, for a fixed center (nucleus), the combination of a magnetic field with the 3d long-range attractive polarization forces lead to an infinite number of bound states for the negative donor^{11,12,13,14}. In two dimensions the long-range interaction is of repulsive character. Indeed, it was shown by Larsen and McCann², that an electron situated far from a 2d D^0 center experiences an overall repulsive potential which prevails both the attractive Coulomb attraction due to the center and the attractive polarization forces. For distances of the order of the extension of the neutral donor, exchange and correlation effects play a major role with respect to the binding mechanism of the additional electron.

Two-dimensional D^- centers in magnetic fields are described by a three-dimensional Schrödinger equation. The finite difference numerical method^{15,16,17,18,19,20,21,22} allows us to solve this Schrödinger equation without any simplifications or approximations with respect to the geometry of the wave function, correlation effects etc. Due to this property of our computational approach it will be here possible to obtain a definite answer on the ground state energy and the number of bound states of the two-dimensional D^- center in magnetic fields. The critical values of the field strengths that are associated with the appearance of the bound states will be determined. One of the major motivations for the present work are the different theoretical values for the ground state energy of a two-dimensional negative donor with and without magnetic field existing in the literature. Variational calculations^{1,3} on the onehand and Monte Carlo simulations⁷ on the otherhand yield incompatible predictions for the ground state energies. This puzzle will be resolved within the present work.

II. THE SCHRÖDINGER EQUATION AND THE METHOD OF SOLUTION

The Hamiltonian of our two-dimensional system of two interacting electrons with an effective mass m and a singly charged positive ion placed into a magnetic field perpendicular to the plane can be written in Cartesian coordinates (x, y) as

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - i\frac{\gamma}{2}\left(-y_1\frac{\partial}{\partial x_1} + x_1\frac{\partial}{\partial y_1} - y_2\frac{\partial}{\partial x_2} + x_2\frac{\partial}{\partial y_2}\right) + \frac{\gamma^2}{8}(r_1^2 + r_2^2) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} \quad (1)$$

Here we use the units $a_{\text{eff}} = \hbar^2 \epsilon \epsilon^{-2} m^{-1} = \epsilon m^{*-1} \cdot 5.29 \times 10^{-9} \text{cm}$ for the length, $E_{\text{eff}} = e^4 \hbar^{-2} m \epsilon^{-2} = m^* \epsilon^{-2} \cdot 27.2 \text{eV}$ for the energy and $B_{\text{eff}} = ce^3 m^2 \hbar^{-3} \epsilon^{-2} = m^{*2} \epsilon^{-2} \cdot 2.3505 \times 10^5 \text{T}$ for the magnetic field strength. $\gamma = B/B_{\text{eff}}$, m_0 is the

mass of the free electron, $m^* = m/m_0$, ϵ is the dielectricity constant of the semiconductor material, $r_1 = (x_1^2 + y_1^2)^{1/2}$, $r_2 = (x_2^2 + y_2^2)^{1/2}$, and $r_{12} = |\vec{r}_1 - \vec{r}_2|$. The spin terms are omitted.

In contrast to variational calculations we are not biased by using a particular ansatz for the variational wave function but will perform a full grid solution to the Schrödinger equation that allows to control and estimate the remaining minor deviation from the exact eigenfunctions and eigenvalues. In the following we provide an outline of our approach which embodies various properties and transformations of the Hamiltonian and the corresponding Schrödinger equation.

Transforming the electronic degrees of freedom to polar coordinates (r_1, ϕ_1) and (r_2, ϕ_2) yields for the Hamiltonian (1)

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial r_1^2} + \frac{1}{r_1} \frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_2} \frac{\partial}{\partial r_2} \right) - \frac{1}{2} \left(\frac{1}{r_1^2} \frac{\partial^2}{\partial \phi_1^2} + \frac{1}{r_2^2} \frac{\partial^2}{\partial \phi_2^2} \right) - i \frac{\gamma}{2} \left(\frac{\partial}{\partial \phi_1} + \frac{\partial}{\partial \phi_2} \right) + \frac{\gamma^2}{8} (r_1^2 + r_2^2) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos(\phi_1 - \phi_2))^{1/2}} \quad (2)$$

The eigenfunctions of this Hamiltonian are the eigenfunctions of the Hamiltonian (1) if we require them to be periodic with period 2π with respect to the variables ϕ_1 and ϕ_2 . The eigenfunctions of the Hamiltonian (2) should also be eigenfunctions of the z -projection of the total orbital angular momentum operator which is a conserved quantity ie. $\mathbf{l}_z \Psi = M \Psi$ with

$$\mathbf{l}_z = -i \frac{\partial}{\partial \phi_1} - i \frac{\partial}{\partial \phi_2} \quad (3)$$

Introducing the coordinates r_1, r_2, ϕ, Φ where

$$\phi = \phi_1 - \phi_2 \quad (4)$$

and

$$\Phi = \frac{\phi_1 + \phi_2}{2} \quad (5)$$

we have

$$\mathbf{l}_z = -i \frac{\partial}{\partial \Phi} \quad (6)$$

For these coordinates the Hamiltonian takes on the appearance

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial r_1^2} + \frac{1}{r_1} \frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_2} \frac{\partial}{\partial r_2} \right) - \frac{1}{8} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{\partial^2}{\partial \Phi^2} - \frac{1}{2} \left(\frac{1}{r_1^2} - \frac{1}{r_2^2} \right) \frac{\partial^2}{\partial \Phi \partial \phi} - \frac{1}{2} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{\partial^2}{\partial \phi^2} - i \frac{\gamma}{2} \frac{\partial}{\partial \Phi} + \frac{\gamma^2}{8} (r_1^2 + r_2^2) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos \phi)^{1/2}} \quad (7)$$

Eigenfunctions of the operator \mathbf{l}_z read as follows

$$\Psi(r_1, r_2, \phi, \Phi) = e^{iM\Phi} \psi(r_1, r_2, \phi) \quad (8)$$

We therefore have

$$H\Psi = e^{iM\Phi} h\psi \quad (9)$$

with

$$h = -\frac{1}{2} \left(\frac{\partial^2}{\partial r_1^2} + \frac{1}{r_1} \frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{1}{r_2} \frac{\partial}{\partial r_2} \right) + \frac{M^2}{8} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) - \frac{iM}{2} \left(\frac{1}{r_1^2} - \frac{1}{r_2^2} \right) \frac{\partial}{\partial \phi} - \frac{1}{2} \left(\frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{\partial^2}{\partial \phi^2} + \frac{M\gamma}{2} + \frac{\gamma^2}{8} (r_1^2 + r_2^2) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos \phi)^{1/2}} \quad (10)$$

This Hamiltonian depends on three degrees of freedom (r_1, r_2, ϕ) and the corresponding Schrödinger equation can therefore be solved for the eigenfunctions and eigenvalues by applying our finite-difference method^{15,16,17}. The coordinates r_1 and r_2 are in the domain

$$0 < r_1 < +\infty, \quad 0 < r_2 < +\infty \quad (11)$$

with zero boundary conditions for infinity. The corresponding domain and boundary conditions for the angle ϕ have to be analyzed in more detail.

From equation (5) one can conclude that solutions of the Schrödinger equation belonging to the Hamiltonian (10) should be considered in the domain $-2\pi \leq \phi \leq 2\pi$ with cyclic boundary conditions. This leads to eigenfunctions that can be either symmetric or antisymmetric with respect to interparticle exchange. The first correspond to spin singlet states whereas the second yield spin triplet states. Beyond this we encounter additional eigenfunctions of the operator (10) that are not eigenfunctions of our initial Hamiltonian (1) i.e. these eigenfunctions do not describe physical solutions. Indeed, exploiting certain symmetries of the wavefunction it is possible to confine the domain of the angle ϕ to $0 \leq \phi \leq 2\pi$ for the Schrödinger equation belonging to the Hamiltonian (10). As a consequence the non-physical solutions are excluded. For the states with $M = 0$ solutions can be obtained in an even smaller domain $0 \leq \phi \leq \pi$.

The numerical finite-difference method employed here to solve the eigenvalue problem for the Hamiltonian (10) is a modification of the approach developed in previous works devoted to atoms in strong magnetic^{17,18,19} and electric fields (see^{20,21} and references therein) and contains, in particular, technical aspects used in three-dimensional problems^{16,22}. Our computational procedure consists of the following main steps. The nodes have to be chosen in the spatial domain $\Omega : 0 \leq r_1 < +\infty, 0 \leq r_2 < +\infty, 0 \leq \phi \leq 2\pi$ (or $0 \leq \phi \leq \pi$). The values of the wavefunctions at the positions of the nodes are the numerical representation of the solutions of the initial differential equations. The nodes of the three-dimensional mesh in the space (r_1, r_2, ϕ) are placed at all the points with coordinates (r_{1i}, r_{2j}, ϕ_k) where r_{1i} , r_{2j} , and ϕ_k are sets of the mesh node coordinates along the corresponding axes. For the coordinate ϕ it is natural to use a uniform mesh with nodes at $\phi_k = 2\pi(k - 1/2)/N$ for the region $0 \leq \phi \leq 2\pi$ (case $M \neq 0$) and $\phi_k = \pi(k - 1/2)/N$ for the region $0 \leq \phi \leq \pi$ (case $M = 0$), where N is the number of nodes in the direction ϕ . For r_1 and r_2 we have used non-uniform distributions of nodes similar to those described in ref.¹⁹, which cover the infinite domains $0 \leq r_1 < +\infty, 0 \leq r_2 < +\infty$ as $N \rightarrow \infty$.

We employ the inverse iteration method to obtain the eigenfunctions and energy eigenvalues. This requires solving a system of linear equations with a matrix that is a finite-difference approximation to the Hamiltonian. The solution of these equations is particularly simple if the matrix has a block-tridiagonal structure. The latter can be achieved using the simplest three-point approximation for the derivatives for one of the coordinates. The choice of this coordinate is dictated by obtaining a convenient form of representation for the boundary conditions. For the two other coordinates we are free to apply more precise higher order approximations to their derivatives. The final values for the energy (and other observables) are provided by using the Richardson extrapolation technique for the corresponding results emerging from a series of geometrically similar meshes with different number of nodes. Using this approach we achieve a major increase of the numerical precision and, in particular, we obtain together with each numerical value a reliable estimate of its precision^{15,17}. Typically, meshes used in the present calculations range from (the sparsest) mesh with 20^3 nodes to (the thickest) one with 38^3 nodes, i.e. 38 nodes in each direction.

III. RESULTS AND DISCUSSION

Our results for the energies of the ground state of the two-dimensional D^- center are presented in table I. This table contains also the corresponding energies for the ground state of the D^0 center and a comparison with the best results obtained in the literature^{2,3,7}. Ref.^{2,3} are variational and ref.⁷ represent Monte-Carlo simulations. One can see, that the variational results by Larsen and McCann coincide for weak and intermediate field strengths³ very well with our results. In contrast to this the results obtained by Louie and Tao Pang⁷ differ significantly from these values. The absence of any approximations in our approach and the possibility to reliably evaluate the convergence of our results allow us to conclude, that the results obtained in ref.⁷ overestimate the true values for the binding energy of the ground state of the two-dimensional negative donor considerably. (The reader should note that all digits of the values for our calculated energies given in table I are converged i.e. coincide with the exact results). This resolves the discrepancy on the ground state energy of the negative donor present in the literature as demonstrated by the results contained in table I particularly for $\gamma = 0$ but also for nonvanishing field strengths.

For strong magnetic fields $\gamma \gg 1$ table I provides also the energies obtained by Larsen and McCann in another variational calculation². Our results both on the total and binding energies show that the ground state of the system is more strongly bound than predicted by ref.². The differences for the energies depend only weakly on the magnetic field strength and are approximately 1.08 a.u. for the total energy and approximately 0.36 a.u. for the binding energy!

TABLE I: D^- donor total and binding energies in two dimensions for the $M = 0$ singlet ground state. Results of our calculations [IS] and refs.^{2,3,7} [other]. The energies of the neutral donor are also given.

| γ | E^{D^-} [IS] | E^{D^-} [other] | E^D [IS] | E^D [other] | $E_B^{D^-}$ [IS] | $E_B^{D^-}$ [other] |
|----------|----------------|-----------------------|------------|--|------------------|---|
| 0 | -2.24027 | -2.239 ³ | -2.00000 | -2.000 ³ -2.000 ⁷ | 0.24027 | 0.239 ³ 0.2555 ⁷ |
| 0.02 | -2.26014 | | -2.009967 | | 0.25017 | |
| 0.05 | -2.28947 | | -2.024869 | | 0.26460 | |
| 0.1 | -2.33712 | | -2.049518 | | 0.28760 | |
| 0.2 | -2.42808 | | -2.098116 | | 0.32996 | |
| 0.5 | -2.67354 | -2.673 ³ | -2.238416 | -2.239 ³ | 0.43512 | 0.435 ³ |
| 1.0 | -3.02151 | -3.021 ³ | -2.455152 | -2.455 ³ -2.455 ⁷ | 0.56636 | 0.566 ³ 0.585 ⁷ |
| 2.0 | -3.58733 | -3.586 ³ | -2.836203 | -2.836 ³ | 0.75113 | 0.750 ³ |
| 3.0 | -4.05355 | | -3.165976 | -3.175 ⁷ | 0.88757 | 0.91 ⁷ |
| 4.0 | -4.45883 | -4.459 ³ | -3.459582 | -3.459 ³ | 0.99925 | 1.000 ³ |
| 10. | -6.27690 | -6.261 ³ | -4.815151 | -4.813 ³ | 1.46175 | 1.463 ³ |
| 20. | -8.36994 | -8.369 ³ | -6.407114 | -6.405 ³ | 1.96283 | 1.964 ³ |
| 50. | -12.5581 | -11.4583 ² | -9.62189 | -8.86227 ² | 2.9362 | 2.5961 ² |
| 100. | -17.2937 | -16.2045 ² | -13.27207 | -12.53314 ² | 4.0216 | 3.6715 ² |
| 200. | -23.9989 | -22.9166 ² | -18.449164 | -17.72454 ² | 5.5497 | 5.1923 ² |
| 500. | -37.3107 | -36.234 ² | -28.737120 | -28.02495 ² | 8.5736 | 8.2097 ² |
| 1000. | -52.316 | -51.243 ² | -40.33926 | -39.63327 ² | 11.977 | 11.610 ² |

TABLE II: Total and binding energies for D^- triplet excited states with $M < 0$.

| γ | $E_{M=-1}^{D^-}$ | E_B | $E_{M=-2}^{D^-}$ | E_B | $E_{M=-3}^{D^-}$ | E_B |
|----------|-----------------------|---------------------|-----------------------|--------------------|-----------------------|---------------------|
| 0.05 | -2.02453 | -0.00034 | -2.02474 | -0.00013 | -2.02481 | -0.00006 |
| 0.1 | -2.0492 | -0.0003 | -2.04916 | -0.00036 | -2.04933 | -0.00019 |
| 0.2 | -2.100 | 0.002 | -2.09715 | -0.00097 | -2.09759 | -0.000528 |
| 0.5 | -2.253 | 0.015 | -2.2360 | -0.0024 | -2.236554 | -0.001862 |
| 1.0 | -2.50275 | 0.04760 | -2.4523 | -0.0029 | -2.4511 | -0.0039 |
| 2.0 | -2.9512 | 0.1150 | -2.83775 | 0.00155 | -2.8302 | -0.0060 |
| 4.0 | -3.68474 | 0.2249 | -3.472622 | 0.01304 | -3.450805 | -0.008773 |
| 10. | -5.2634 | 0.4482 | -4.85787 | 0.04272 | -4.796 | -0.019 |
| 20. | -7.1028 | 0.6957 | -6.4853 | 0.0782 | -6.381 | -0.026 |
| 50. | -10.80161 | 1.17972 | -9.7707 | 0.1488 | -9.590 | -0.032 |
| 100. | -14.99309 | 1.72102 | -13.501 | 0.229 | -13.236 | -0.036 |
| 200. | -20.933 | 2.484 | -18.794 | 0.345 | -18.41 | -0.04 |
| 500. | -32.732 | 3.995 | -29.25 | 0.51 | -28.69 | -0.05 |
| 500. | -32.1289 ² | 4.1009 ² | -28.6261 ² | 0.602 ² | -28.0464 ² | +0.021 ² |

The significant difference in deviations of our results from those obtained in ref.² is due to the fact that the binding energies of the neutral donor in a strong magnetic field are underestimated in ref.². As shown below this leads also to an overestimation of the binding properties of the excited states of the D^- center.

The ground state of the D^- center is the only bound state for $\gamma = 0$. We have carried out calculations for excited states of both symmetric and antisymmetric character of the spatial wavefunction with respect to the interchange of the coordinates of the electrons (i.e. spin singlet and triplet states). These calculations were implemented both for $M = 0$ and for $M \neq 0$. The latter states were investigated also by Larsen and McCann². Without loss of generality we confine ourselves to negative magnetic quantum numbers $M < 0$. Pairs of states being different only with respect to the sign of M possess equal binding energies within the corresponding Landau zones. However, opposite to states with negative M , states with $M > 0$ do not belong to the lowest Landau zone. Therefore, it is reasonable to focus on

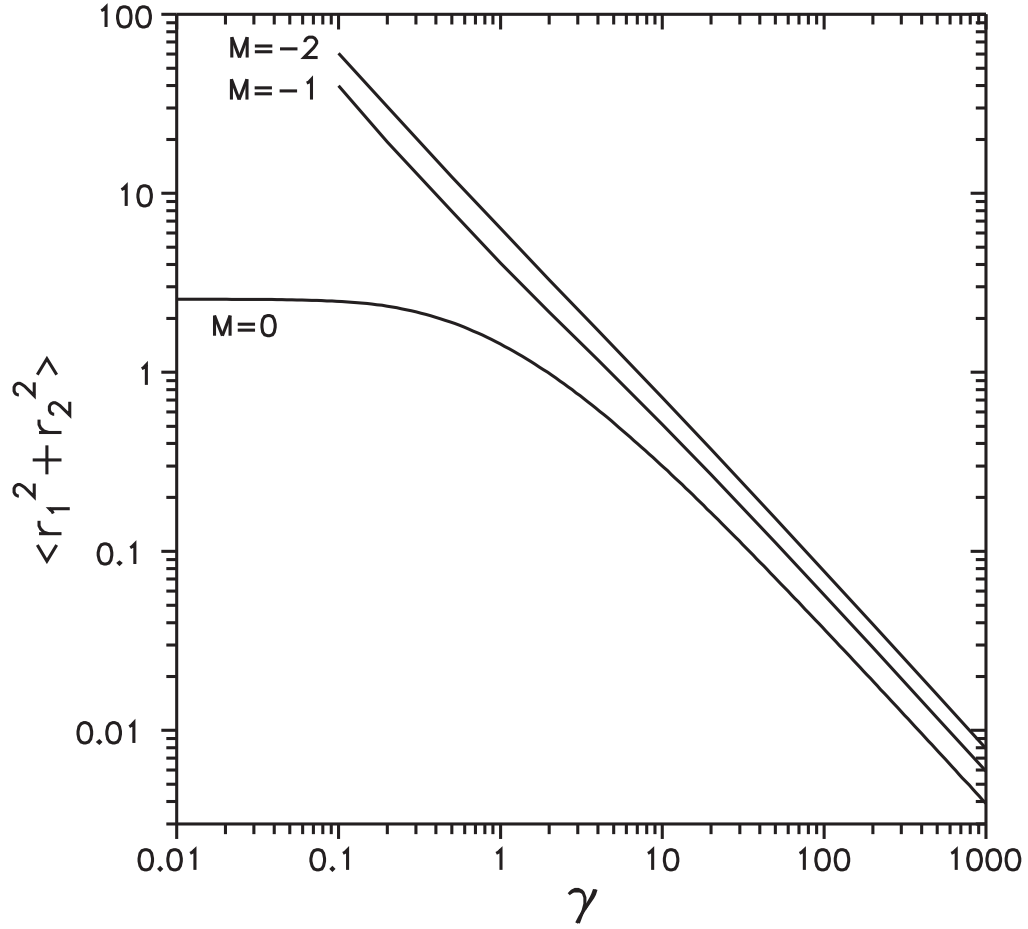


FIG. 1: $\langle r_1^2 + r_2^2 \rangle$ depending on the magnetic field strength for the three lowest states of the two-dimensional D^- center. Effective atomic units are used (see text).

values $M \leq 0$.

Our calculations show that the ground state of the D^- center is the only spin singlet state which is bound in the presence of magnetic fields. This conclusion coincides with results obtained in ref.². On the otherhand, it follows from our calculations of the triplet states (see table II) that there are two triplet states that become bound above some corresponding critical values for γ . These are the energetically lowest states for $M = -1$ and $M = -2$, respectively. The $M = -1$ state becomes bound for $\gamma > 0.117$ (the total energy of both D and D^- at $\gamma = 0.117$ is -2.057852). The state with $M = -2$ becomes bound for $\gamma > 1.68$ (the total energy at $\gamma = 1.68$ is -2.720788).

From table II it is evident that the lowest state with magnetic quantum number $M = -3$ is not bound for any magnetic field strength considered here and probably also for higher field strengths (the binding energy $E_B = E^D - E^{D^-}$ is negative and its absolute value increases with increasing field strength). This result differs from that obtained by Larsen and McCann². They received a positive binding energies for this state for sufficiently strong magnetic fields. Their binding energy for $\gamma = 500$ is presented in the last row of table II. The main reason for this discrepancy is the underestimation of the binding energy of the neutral donor in ref.² as can be seen from table I. The data of table II together with our results for other excited states (they are unbound) allow us to conclude that the D^- considered possesses only two bound excited states – possessing magnetic quantum numbers $M = -1$ and $M = -2$.

Along with the total and binding energies of the two-dimensional negative donor D^- we have calculated some geometrical parameters of its wavefunction that provide additional information about the system. In figure 1 we present the expectation value $R^2 = \langle r_1^2 + r_2^2 \rangle$ which characterize the extension of the spatial distribution of the electrons in the simplest and most straightforward way as a function of the field strength. First of all we observe that the electronic cloud is shrinking monotonically with increasing field strength for all bound states. This had to expected according to what we know about the behaviour of tightly bound states of few-electron system in strong magnetic fields²¹. The difference of the behavior of R^2 for the ground ($M = 0$) and excited ($M \neq 0$) states for

relatively weak magnetic fields is obvious: The ground state is bound for $\gamma = 0$, its wave function remains localized for all values of γ , and R^2 possesses a finite limit for $\gamma \rightarrow 0$. Furthermore it changes little for $\gamma \leq 0.1 a.u.$ For the excited states R^2 is not bounded for $\gamma \rightarrow 0$. It changes rapidly with increasing field strength in particular in the weak magnetic field regime. Therefore R^2 possesses finite values for excited states only due to the presence of the magnetic field. On the otherhand, the dependencies of R^2 on the magnetic field strength in the high field regime are similar for all considered states since they are dominated by the diamagnetic term $\gamma(r_1^2 + r_2^2)/8$ of the Hamiltonian. The occurrence of a small curvature in the dependence $R^2(\gamma)$ for $M = -1$ between $\gamma = 0.1$ and $\gamma = 10$ is due to the influence of internal binding forces of the system, which are not negligibly small compared to the magnetic forces for this range of field strengths.

IV. BRIEF SUMMARY

We have shown that the two-dimensional negative donor D^- possesses three bound states ie. two bound excited states in the presence of a sufficiently strong magnetic field. The spin singlet ground state is bound for arbitrary field strengths. Our investigation of the ground state clarifies a discrepancy in the literature and confirms previous variational calculations^{1,3}. As a result the energy eigenvalues obtained in ref.⁷ turn out to violate the variational principle and are too low i.e. the corresponding binding energies are too large. For weak and intermediate field strength we obtain good agreement of our total and binding energies compared to those of ref.³. In the high field regime, however, a significant lowering of the total energies and raising of the binding energies are obtained within the present investigation. Our particular computational approach allows for an estimate of the difference of our (up to several digits converged) results and the exact ones which consequently allows us to draw definite conclusions on the energies and properties of the donor. A series of calculations for excited states show that two other states become bound with increasing magnetic field strength. They are the lowest excited states with $M = -1$ ($\gamma > 0.117$) and $M = -2$ ($\gamma > 1.68$). The extension of these states decreases monotonically with increasing field strength.

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- * Electronic address: mivanov@mi1596.spb.edu; Permanent address: Institute of Precambrian Geology and Geochronology, Russian Academy of Sciences, Nab. Makarova 2, St. Petersburg 199034, Russia
- † Electronic address: Peter.Schmelcher@tc.pci.uni-heidelberg.de
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